X-ray Fluorescence Measurements of Irradiated Polymer Films and Organic Superconductors

E.Z.Kurmaev[1], R.Winarski[3], A.Moewes[3], D.L.Ederer[2], A.I.Poteryaev[1], K.Endo[4], T.Ida[4], J.-C.Pivin[5],G.S.Chang[6], B.Schneider[7], M.Neumann[7], and C.N.Whang[6]

[1]*Institute of Metal Physics, Russian Academy of Sciences-Ural Division, 620219 Yekaterinburg GSP-170, Russia*

[3]*Department of Physics, Tulane University, New Orleans,LA 70118, USA*

[3]*Center for Advanced Microstructures and Devices, CAMD at Louisiana State University, Baton Rouge, LA 70803*

[4]*Department of Chemistry, Faculty of Science, Kanazawa University, Kanazawa, Japan*

[5]*CSNM, Bat. 108, 91405 Orsay Campus, France*

[6]*Department of Physics, ASSRC, Yonsei University, Seoul 120-749, Korea*

[7]*University of Osnabrück, Department of Physics, D-49069, Germany*

Fluorescent X-ray *C Kα* and *O Kα* emission spectra (XES) have been measured to study the electronic structure of polyimide films (PMDA-ODA) prepared by the spin-coating method and ionized cluster-beam deposition on the Si-substrate. We found that the spectral emission features are not changed when the time of exposure was increased from 600 to 1800 sec. This indicates that polyimide films are rather stable to the exposure of monochromatic synchrotron radiation and the experimental fluorescent *C Kα* and *O Kα* XES can be used for the analysis of the electronic structure of polyimide films. The occupied states of PMDA-ODA have also been investigated and compared with molecular orbital calculations of the model monomer containing 41 atoms using a semi-empirical Hydrogenic atoms in molecules version 3 (HAM/3) method. From the comparison of our calculations with the experimental results we identify the origin of the spectral features and find excellent agreement [1].

We have used fluorescent *C Kα* XES to characterize the bonding of carbon atoms in irradiated polyimide (PI) and polycarbosilane (PCS) films. The PI films have been irradiated with 40 keV N_2^+ or Ar^+ ions, at fluences ranging from $1x10^{14}$ to $1x10^{16}$ cm^{-2}. The PCS films have been irradiated with $5x10^{15}$ C^+ ions cm^{-2} of 500 keV and/or annealed at 1000^0 C. We find that the fine structure of the carbon XES of the PI films changes with implanted ion fluence above $1x10^{14}$ cm^{-2}. This is attributed to the degradation of the PI into amorphous C:N:O. The bonding configuration of free carbon precipitates embedded in amorphous SiC, which are formed in PCS after irradiation with C^+ ions or combined treatments, is close to either that one in diamond-like films or the one in silicidated graphite [2].

We have measured X-ray fluorescent *S* $L_{2,3}$, *C Kα* and *N Kα* XES of superconducting inorganic polymer single crystals $(SN)_x$ and $(ET)_4Hg_{2.89}Br_8$ and compared the results of the XPS and UPS measurements with our self-consistent *LMTO-TB* band structure calculations. The orbital composition of the energy bands of $(SN)_x$ and $(ET)_4Hg_{2.89}Br_8$ is analyzed. The electronic states that dominate the density of states near the Fermi level are determined.

This work was supported by the Russian State Program on Superconductivity, the Russian Science Foundation for Fundamental Research (Project 96-15-96598, 97-03-33686a and 98-02-04129), the NATO Linkage Grant (HTECH.LG 971222) and the DFG-RFFI Project.

[1] R.P.Winarski, D.L.Ederer, E.Z.Kurmaev, S.N.Shamin, K.Endo, T.Ida, A.Moewes, G.S.Chang, S.Y.Kim and C.N.Whang (Thin Solid Films, in press).
[2] R.P.Winarski, D.L.Ederer, J.-C.Pivin, E.Z.Kurmaev, S.N.Shamin, A.Moewes, G.S.Chang, C.N.Whang, K.Endo, T.Ida, Nucl. Instr. Meth. B 145, 401 (1998).
[3] E.Z.Kurmaev, A.I.Poteryaev, V.I.Anisimov, I.Karla, A.Moewes, B.Schneider, M.Neumann, D.L.Ederer, R.N.Lyubovskaya (subm. to PRB).

Principal investigator: Ernst Z. Kurmaev, Institute of Metal Physics, Russian Academy of Sciences–Ural Division. Email: kurmaev@ifmlrs.intec.ru. Telephone: 7-3432-744183.